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MS-12-P-3263 Study of structural defects in Fe₃O₄ thin films: atomic scale correlation between imaging and spin calculations

Gilks D.¹, Evans R.¹, Matsuzaki K.², McKenna K.¹, Lari L.^{1,3}, Susaki T.², Lazarov V. K.¹

¹Department of Physics, University of York, Heslington, York, YO10 5DD, UK, ²Secure Materials Center, Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, ³York JEOL Nanocentre, University of York, Heslington, York, YO10 5BR, UK

Email of the presenting author: dg522@york.ac.uk

Bulk Fe₃O₄ exhibits many of the properties required for spintronic device applications. First principle calculations predict Fe₃O₄ is a halfmetal with only minority spin density states at the Fermi level [1]. Furthermore, Fe₃O₄ has a high Curie temperature of ~868K. Good epitaxy between Fe₃O₄ and current oxide barrier materials such as MgO and MgAl₂O₄ makes realistic spin devices based on halfmetals viable. However, extended growth defects known as anti-phase domain boundaries (APB) frequently found in Fe₃O₄ films (Figure 1) have a significant impact on the magnetic properties of grown films [2]. To utilize the halfmetallic properties of Fe₃O₄ we must understand how the presence of various defects affects the magnetic properties and spin dynamics in grown films.

In Fe₃O₄, O mediates super exchange interactions between the magnetic Fe sites. Such interactions are dependent on both bond length and angle in the various Fe-O-Fe configurations observed in Fe₃O₄. These short range interactions are dominated by the co-ordination of nearest neighbour Fe sites [3] thus requiring accurate atomistic models to begin to understand APB defects.

In order to simulate the magnetic behaviour of APBs, atomistic models of APB defects have been produced using atomically resolved HAADF STEM images (Figure 2) and image simulations to verify realistic structures.

From this we simulate the magnetisation curves (figure 3a) and the Curie temperature (Figure 3b) of Fe₃O₄ using super cells containing over 10000 individual spins. This allows us to consider the effective atomistic Heisenberg interactions which act between neighbouring Fe sites, both at and away from a two dimensional defect.

1. Yanase, A. and K. Siratori, Band-Structure in the High-Temperature Phase of Fe₃O₄. Journal of the Physical Society of Japan, 1984. 53(1): p. 312-317.
2. Margulies, D.T., et al., Origin of the Anomalous Magnetic Behavior in Single Crystal Fe₃O₄ Films. Physical Review Letters, 1997. 79(25): p. 5162-5165.
3. Wickham, D.G. and J.B. Goodenough, Suggestion Concerning Magnetic Interactions in Spinels. Physical Review, 1959. 115(5): p. 1156-1158.

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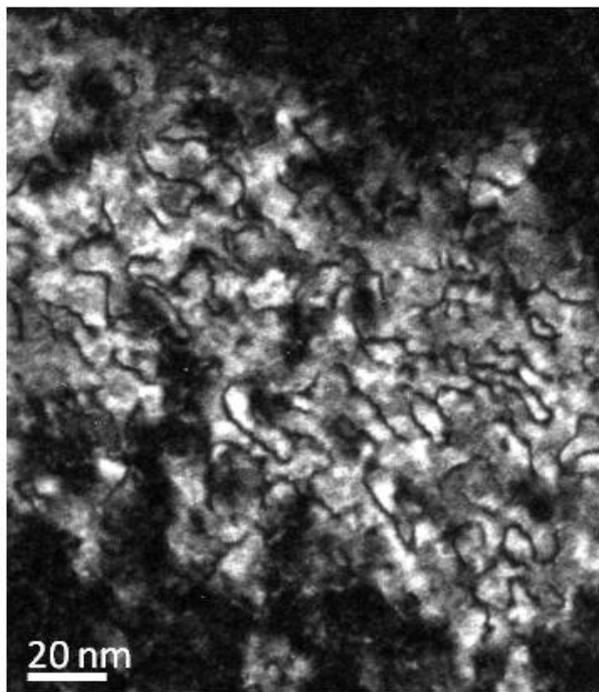


Fig. 1: DF-TEM image of APBs imaged in plan view geometry from a (001) oriented Fe_3O_4 film

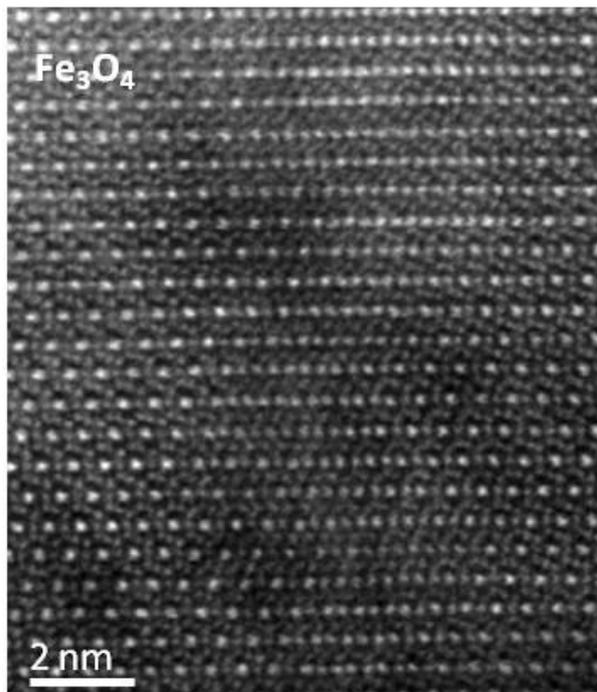


Fig. 2: HAADF-STEM image of an APB running vertically through a (111) oriented Fe_3O_4 film. This APB can clearly be seen in the centre of the image where the rhombohedral structural motif seen to the left and right of the image is lost.

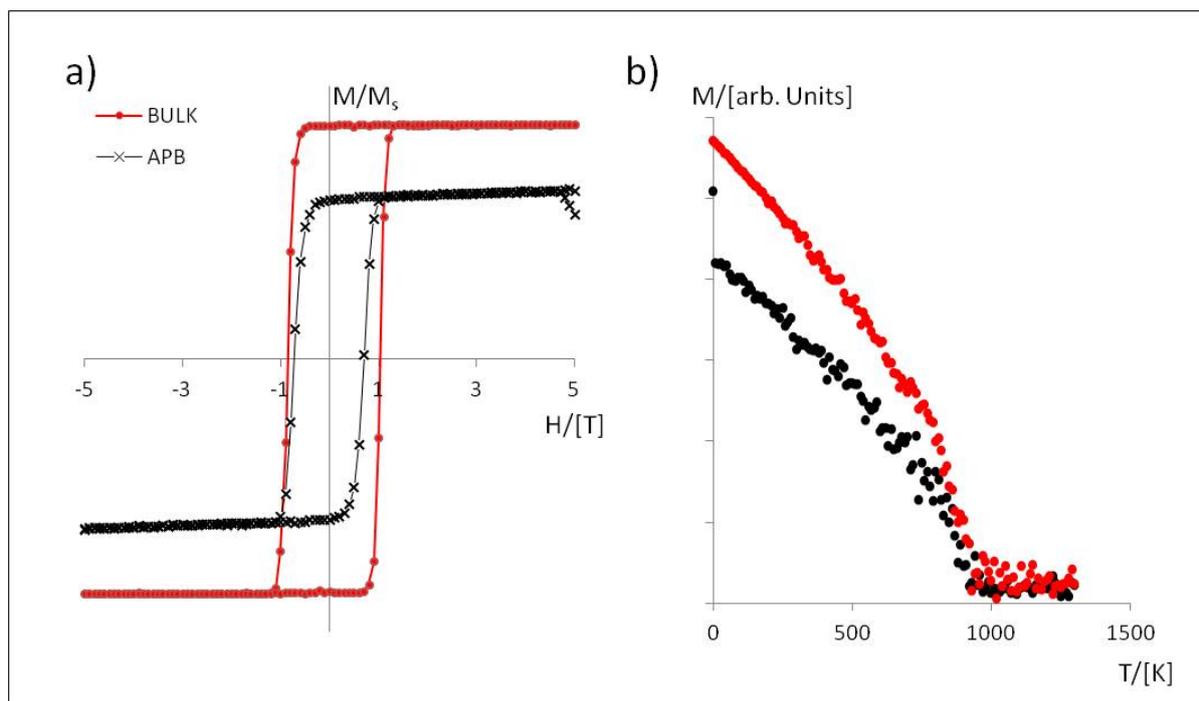


Fig. 3: Magnetic simulation from bulk Fe_3O_4 and a region containing an APB. (a) shows the simulated M-H curves for the APB model (red) and the bulk model (black). (b) shows the Curie temperature measurements.